A level coupled to a 1D interacting reservoir : A DMRG study

M. Sade, Y. Weiss, M. Goldstein and R. Berkovits[1]

[1]*The Minerva Center, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel*

The influence of interactions in a reservoir coupled to a level on the width of the filling as a function of the chemical potential and the position of the level is studied. The density matrix renormalization group (DMRG) method is used to calculate the ground state of a finite-size interacting reservoir, linked to a single state dot. The influence of the interactions in the lead as well as dot-lead interactions is considered. It is found that interactions in the reservoir result in a decrease in the resonance width, while the dot-lead interaction has an opposite effect. These effects are explained within the random phase approximation as an effective change in the inverse compressibility of the reservoir, while the dot-lead interactions renormalize the position of the level.

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There has been much interest in the conduction through a 1D interacting system, especially in clarifying the behavior of a Luttinger liquid with impurities[1]. Essentially, it was shown that any impurity will lead to an insulating behavior. The resonance conductance through a quantum dot coupled to a pair of Luttinger liquid leads (see Fig. 1a) was found to produce infinitely sharp Coulomb blockade peaks at zero temperature[2]. Thus, no level broadening of the dot states is exhibited in the measurement of the conduction through that dot.

Nevertheless, this does not imply that coupling a dot to a Luttinger liquid has no effect on the width of the filling as a function of the chemical potential. Consider for example the arrangement depicted in Fig. 1b. A dot is connected to a Luttinger liquid lead, while its occupation is measured by a quantum point contact (QPC). Thus, the Luttinger liquid acts as a reservoir for the dot, while the QPC is used to probe the dots level broadening. In such an arrangement, any additional broadening of the levels due to the coupling to the reservoir will be seen in the shape of the conductance through the QPC.

The difference between the two arrangements is that while the first case (Fig. 1a) essentially probes the enhancement of the backscattering in the Luttinger liquid in the vicinity of the Fermi energy, the second (Fig. 1b) explores the broadening of the level due to coupling to states which may be far from the Fermi energy. Therefore, one might expect the broadening of the level measured in the second arrangement to approach the conventional Briet-Wigner form, although some signature of the interactions is anticipated.

In this paper we study the broadening of a level coupled to a Luttinger liquid reservoir (Fig. 1b). We use the numerical density matrix renormalization group (DMRG)[3] in order to calculate the ground state of the dot-lead system for spinless interacting electrons. It will be shown that the level broadening even for an interacting lead is well described by the Briet-Wigner form. Despite that, the interactions in the lead leave a clear signature in the broadening of the level. If there is no electrostatic coupling between the dot and lead, the interactions in the lead result in a reduced width of the level. On the other hand, such electrostatic coupling leads to an increase in the width as well as to a change in the levels' energy.

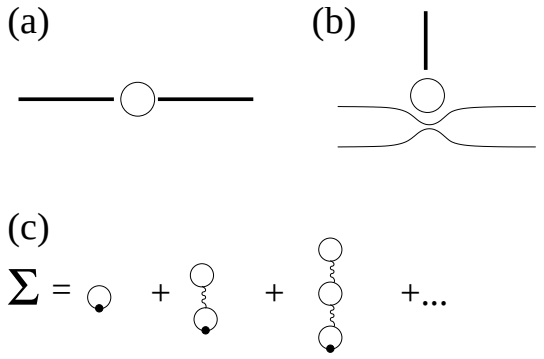

FIG. 1: (a) A level (quantum dot) coupled to two Luttinger liquid leads represented by the wide lines. (b) A level coupled electrostatically to a QPC through which the conductance in measured, and to an interacting reservoir. (c) The diagrammatic representation of the RPA approximation of the self energy. The line corresponds to the lead Green function, the black dot to the hopping into the dot and the wiggly line to the interaction.

The DMRG method is used to calculate the orbital population in a system consisting of a one-orbital dot coupled to an interacting lead. At the first stage interactions between the dot and the lead are not taken into account. The Hamiltonian describing the system is therefore given by:

$$\hat{H} = \epsilon_0 \hat{a}^\dagger \hat{a} - V(\hat{a}^\dagger \hat{c}_1 + \hat{c}_1^\dagger \hat{a}) - t \sum_{j=1}^{N-1} (\hat{c}_j^\dagger \hat{c}_{j+1} + h.c.) + I \sum_{j=1}^{N-1} (\hat{c}_j^\dagger \hat{c}_j \hat{c}_{j+1}^\dagger \hat{c}_{j+1}), \quad (1)$$

where ϵ_0 is the dot's orbital energy level, V (t) is the dot-lead (lead) hopping matrix element, and I is the nearest-neighbor interaction strength in the lead. $\hat{a}^\dagger$ $(\hat{a})$ is the creation (annihilation) operator of an electron in the dot, and $\hat{c}_j^\dagger$ $(\hat{c}_j)$ is the creation (annihilation) operator of an electron at site j in the lead.

The Hamiltonian H was diagonalized using a finite-size DMRG calculation[3,4] for a lead of 150 sites, and $n(\mu)$ curves were calculated for several coupling strengths, V, and interaction strengths, I. The lead hopping element, t, is taken as 1, in order to set the energy scale.

Typical results for $n(\mu)$ are shown in Fig. 2. As can be seen, increasing the interaction strength in the lead (I) results in a decrease of the level width, while almost no shift in the level position occurs.

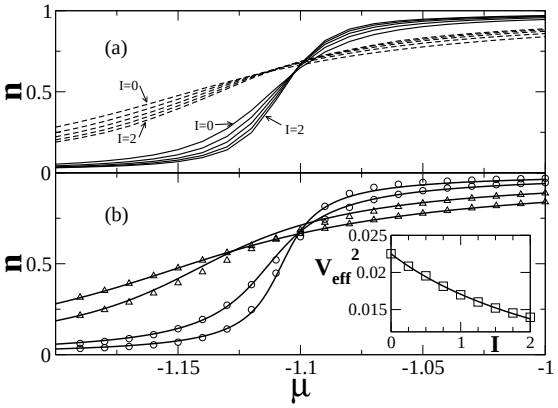

FIG. 2: (a) The dot's population as a function of the chemical potential for different interaction strengths. The full lines represents results for lead-dot coupling $V = 0.15$, and the dashed lines for $V = 0.3$. In both cases the interaction strength I takes values between 0 and 2, in jumps of 0.5. (b) The same plots for $I = 0$ and 2 are drawn again ($V = 0.15$ in circles, $V = 0.3$ in triangles) together with theoretical fits using Eq.(6) (lines). Inset: V_{eff}^2 as a function of I (symbols) as obtained by fitting the $n(\mu)$ curves of $V = 0.15$ to Eq.(6). The line corresponds to the dependence according to Eq.(8).

In order to estimate the influence of the interactions in the lead on the shape of $n(\mu)$, one should start from considering the non-interacting case. The coupling of the dot state to the continuum (akin to the Fano-Anderson model) may be treated using standard Green function technique[5] which leads to:

$$n_{dot}(\mu) = \frac{1}{\pi}\int_{-\infty}^{\mu} \frac{\Im\Sigma(\epsilon)}{(\epsilon - \epsilon_0 - \Re\Sigma(\epsilon))^2 + (\Im\Sigma(\epsilon))^2} d\epsilon, \quad (2)$$

where $\Sigma(\epsilon)$ is the self energy given by:

$$\Sigma(\epsilon) = \sum_k \frac{|V_k|^2}{\epsilon - \epsilon_k - i\delta}, \quad (3)$$

ϵ_k are the eigenvalues of the lead, V_k is the coupling between the eigenstates in the lead and the state in the dot and $\delta \to 0$.

For the idealized case, the density of states in the lead is constant (i.e., $\epsilon_k = k/L\nu$, where ν is the (constant) local density of states, and L is the leads length). The coupling is $V_k = \sqrt{a/L}V$ (a is the nearest neighbor distance), and under these conditions

$$\Sigma(\epsilon) = \frac{a}{L}\int \frac{|V|^2 dk}{\epsilon - k/L\nu - i\delta}, \quad (4)$$

resulting in $\Im\Sigma(\epsilon) = \pi a\nu|V|^2 = \Gamma/2$ and $\Re\Sigma(\epsilon) = 0$. Thus, one obtains the Breit-Wigner formula:

$$n_{dot}(\mu) = \frac{1}{\pi}\int_{-\infty}^{\mu} \frac{\frac{\Gamma}{2}}{(\epsilon - \epsilon_0)^2 + (\frac{\Gamma}{2})^2} d\epsilon. \quad (5)$$

For the tight-binding model given in Eq.(1), $\epsilon_k = -2t\cos(ka)$ and $V_k = \sqrt{2a/L}\sin(ka)V$, resulting in $\Im\Sigma(\epsilon) = (V^2/t)\sqrt{1-(\epsilon/2t)^2}$ and $\Re\Sigma(\epsilon) = (V/t)^2\epsilon/2$. We thus find

$$n_{dot}(\mu) = \frac{1}{\pi}\int_{-2}^{\mu} \frac{\frac{V^2}{t}\sqrt{1-\frac{\epsilon^2}{4t^2}}}{\frac{V^4}{t^2}(1-\frac{\epsilon^2}{4t^2}) + ((1-\frac{V^2}{2t^2})\epsilon - \epsilon_0)^2} d\epsilon. \quad (6)$$

We shall now turn to discuss the role played by interactions in the lead. It is well known that the excitations in the vicinity of the Fermi energy of any 1D interacting system should be described as a Luttinger liquid. Nevertheless, the dot occupation $n_{dot}(\mu)$ is determined by contributions from all energies, and the region around the Fermi energy does not play a unique role. Therefore, one could expect a simple perturbation description of the interactions in the lead to suffice. Indeed, the effect of the e-e interactions in the RPA approximation on the self energy (see Fig. 1c) may be written as[6]:

$$\Sigma(\epsilon) = \chi\Sigma^0(\epsilon) \quad (7)$$

where $\Sigma^0(\epsilon)$ is the non-interacting self energy and

$$\chi = \frac{1}{1 + a\nu I}. \quad (8)$$

Here we assumed a constant local density of states ν (for the tight binding lead $\nu = (a\pi t)^{-1}$ which ignores local density of states variations), thus one obtains $\Im\Sigma(\epsilon) = (V^2/t(1 + I/\pi t))\sqrt{1-(\epsilon/2t)^2}$ and $\Re\Sigma(\epsilon) = (V^2/t(1 + I/\pi t))\epsilon/2$, corresponding to replacing V^2 in Eq.(6) by an "effective" coupling $V_{eff}^2 = V^2(1 + I/\pi t)$.

Returning to the results obtained by the numerical DMRG calculations, the curves of Fig. 2 can be now fitted to Eq.(6) with two fitting parameters - $\epsilon_{0,eff}$ and V_{eff}^2. It is easy to see that the Briet-Wigner form fits quite well even in the presence of strong interactions. The effect of interactions is limited here to a decrease of V_{eff}^2, i.e., decrease of Γ, while the level position $\epsilon_{0,eff} = \epsilon_0$ remains constant. The values of V_{eff}^2 extracted from the fit are plotted in Fig. 2(inset) and compared with the RPA predictions of $V_{eff}^2 = V^2(1 + I/\pi t)$. A rather good correspondence is observed.

In order to consider interactions between an electron occupying the dot, and the electrons in the lead, an additional interaction term should be added to the Hamiltonian (Eq. (1)):

$$\hat{H}_{dl} = I_{dl}\hat{a}^{\dagger}\hat{a}\hat{c}_1^{\dagger}\hat{c}_1. \quad (9)$$

DMRG calculations were performed for $H + H_{dl}$, and the corresponding $n(\mu)$ results (Fig. 3) clearly show a change in the resonance width, but also a change in the level position, which was absent in the previous case. Nevertheless, these results can still be fitted to Eq.(6) with the same fitting parameters - $\epsilon_{0,eff}$ and V^2_{eff}. As can be seen, Eq.(6) describes this system quite well.

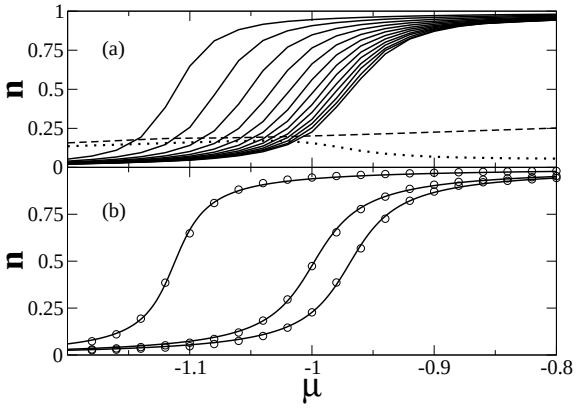

FIG. 3: (a) Population of the dot and of the first site of the lead as a function of the chemical potential, for $V = 0.15$. Dot-lead interaction was included (Eq.(9)) taking $I_{dl} = I$. The curves shown are for I between 0 and 3, in jumps of 0.25 (full lines, dot population), and for $I = 0$ (dashed line) and $I = 2$ (dotted line) for the lead population. (b) The plots for $I = 0, 1.5$ and 3 (symbols) together with the best fit to Eq.(6).

The resonance center movement, $\epsilon_{0,eff}$, as well as the width, V^2_{eff}, that were obtained from the fit can be seen in Fig. 4. For small values of interaction both grow linearly. First lets try to explain the shift in the resonance center. As noted, almost no shift was seen for $I_{dl} = 0$. In the presence of weak dot-lead interactions, one may approximate $\hat{H}_{dl} \sim I_{dl}n_1\hat{a}^{\dagger}\hat{a}$, where n_1 represents the average occupation of the first site in the lead. As can be seen in Fig. 3a, n_1 is not very sensitive to the occupation of the dot and may be replaced by its typical value. Thus, the energy of the orbital in Eq.(1) may be rewritten as $\epsilon_{0,eff} = \epsilon_0 + n_1 I_{dl}$. Indeed, this formula fits well the numerical results for small values of I_{dl} (as can be seen in Fig. 4(a)), for $n_1 = 0.14$. This result agrees well with the value $n_1 \sim 0.15$ in the region of the resonance, taken from the data of Fig. 3(a).

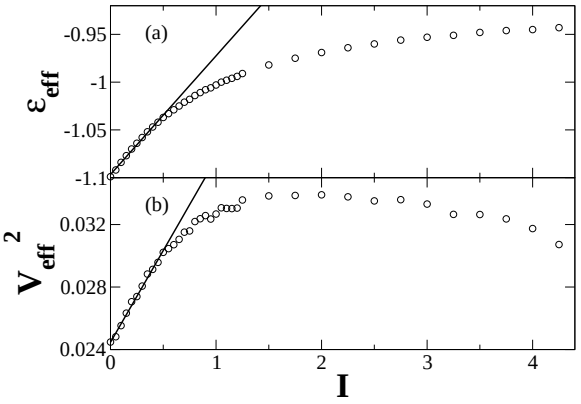

FIG. 4: (a) $\epsilon_{0,eff}$ and (b) V^2_{eff} as functions of $I_{dl} = I$ for $V = 0.15$ (symbols) and linear fits for the region $I \leq 0.5$ (lines).

A more striking feature is the behavior of V^2_{eff}, i.e, the width of the resonance. There is a distinct qualitative change in the width behavior, compared to the case without dot-lead interactions. As opposed to the monotonic decrease of V^2_{eff}, which was demonstrated in Fig. 2 (inset), Fig. 4b (symbols) shows that V^2_{eff} increases with I, until a maximal value is achieved around $I = 2$. For larger values of interaction decrease in the width is observed.

This enhancement of V^2_{eff} is associated to the interplay between the population of the dot level to the depopulation of the first site in the lead, ignored in our treatment of $\epsilon_{0,eff}$. This leads to a reduction in the effect of the dot-lead interaction which results in an increase in the width as depicted in Fig. 4b. For weak interactions the enhancement of V^2_{eff} is linear.

Thus, although the Luttinger liquid has a vanishing local DOS at the end of the lead in the vicinity of the Fermi energy, a level coupled to a 1D interacting reservoir is broadened, since all the reservoir states take part in the broadening mechanism. Nevertheless, as we have seen, the interactions in the reservoir influence the width of the resonance. One might gain some insight from the following consideration: For the non-interacting case (for constant density of states in the reservoir) the width is equal to $\Gamma = 2\pi a\nu|V|^2$, which may be rewritten as $\Gamma = 2\pi(a/L)|V|^2\partial N/\partial\mu$. The thermodynamic inverse compressibility $\partial N/\partial\mu$ is affected by the interactions[7].

Lets consider the compressibility $\partial\mu/\partial N$. In the lowest order approximation[6] $\partial\mu/\partial N = (L\nu)^{-1} + e^2/C$, where C is the capacitance of the system. For nearest neighbor interaction $e^2 = aI$ and as usual $C \sim L$. Therefore, $\partial N/\partial\mu = L\nu/(1 + a\nu I)$. Inserting this to the expression for Γ, we get a result similar to the RPA approximation results in Eq.(8). Although capacitance is proportional to the length L of the lead, so is the density of states in a 1D system, and therefore it has an influence even for an infinite lead.

The conductance through the QPC in the geometry described in Fig. 1b is directly proportional to the occupation of the dots' orbital due to the capacitive coupling between the charge of the dot and the QPC (it is assumed that no tunneling occurs between the dot and the QPC)[8]. Thus, in principal, $n_{dot}(\mu)$, may be read off the conductance through the QPC and the effect of coupling of the dot to the interacting reservoir can be measured.

In conclusion, interactions in a reservoir coupled to a resonant level leave clear fingerprints on the width and position of the resonance. The main influence is the decrease in the resonance width due to a change in the inverse compressibility of the reservoir. On the other hand, the dot-lead interaction shifts the resonance position and may also enhance the width.

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